DSSTox Log File:

EPA Integrated Risk Information System (IRIS) Toxicity Review Data (IRISTR)

(last updated 19 February 2008)

Description: Information in this file documents the creation, review, and update process for the DSSTox IRISTR SDF (Structure Data Format) file and provides summary information on data file content. The first section summarizes the process used for creating the initial DSSTox SDF files, and the quality assurance checks and procedures employed. A table providing field and data counts offers summary overview of IRISTR file contents and chemical composition. The Log Table documents modifications and revisions to the database content or format in version updates. To obtain the most current version of this Log File and a record of any new modifications, a user should consult the DSSTox IRISTR database page: http://www.epa.gov/ncct/dsstox/sdf_iristr.html

QA and Development Notes for IRISSI_v1a:
IRISTR_v1a is an expanded and modified version of the original EPA IRIS Structure-Index (IRISSI_v1a) file published in April 2006. The IRISSI_v1a SDF file underwent an extensive series of quality review checks prior to publication of the initial launch version. The original IRISSI_v1a Structure-Index file was created from the chemical listing provided on the EPA IRIS Source website (http://www.epa.gov/iris/subst/index.html), with URL addresses linking to IRIS QuickView documents for all substances extracted from the html IRIS chemical listing page through an automated Python script (written by Jamie Burch). IRIS chemical names and CAS registry numbers were checked for internal consistency prior to chemical structure assignment following current Chemical Information Quality Review Procedures (see http://www.epa.gov/ncct/dsstox/ChemicalInfQAProcedures.html). Based initially on CASRN matching, DSSTox Standard Chemical Fields were populated from the DSSTox Master File content, with remaining chemical information populated from a variety of commercial and public resources.

QA and Development Notes for IRISTR_v1a:
Changes to DSSTox Standard Chemical Fields from IRISSI_v1a to IRISTR_v1a include new ID fields: **DSSTox_RID**, **DSSTox_Generic_SID** and **DSSTox_FileID** (replacing **DSSTox_SID** and **DSSTox_ID_FileName**) (see http://www.epa.gov/ncct/dsstox/MoreonStandardChemFields.html). Also, entries in the **TestSubstance_Description** field have been simplified. The most substantive changes in IRISTR_v1a are the addition of 3 Standard Toxicity Fields (**StudyType**, **Endpoint**, **Species**) and 33 Source-specific toxicity content fields for 5 IRIS toxicity review assessment areas, the latter generated from automated search outputs available on the EPA IRIS website.

Most of the IRISTR Source-Specific Fields were directly extracted from the EPA IRIS Source Website in Oct 2006 using the "Multiple Substance Report" page (left side-bar link on the IRIS Home page): all chemical substances in the "Select Multiple Substances" window were selected; and all 5 "types of data to compare", or toxicity review areas, were selected (Oral RfDs, Inhalation RfCs, Weight of Evidence Characterizations, Oral Slope Factors/Drinking Water Risks, Air Unit Risks). Clicking on "Generate a Web Report" generated several html tables, one corresponding to each toxicity review area, which were subsequently transferred to a single Excel data table. These data underwent extensive cleaning and modification to standardize, simplify, and create more consistent text entries and notations. Changes included: conversion of all quantitative information fields (Oral RfDs, Inhalation RfCs, etc) to pure numeric form; conversion of mg unit fields to mmol unit fields; addition of integer "count" fields for each toxicity review assessment area (to enable quick counting and extraction of the subset of substances evaluated in each of the 5 toxicity review areas); elimination of abbreviations and footnotes; and some editing and standardization of "Critical Effects" and "Precursor Effect/Tumor Type" field entries to be more consistent throughout the file. The purpose of these changes is not to replace the content of the IRIS Summary documents, which include substantial details and descriptive information. Rather, through import of the SDF file into specialized applications, the goal is to make portions of IRIS data more available and useful in relational database and chemical searching applications, and to include IRIS data in larger aggregations and compilations of toxicity data. The original IRIS output categories and column headers, and any modifications to the original IRIS data are documented in the ***Comments*** column of the IRISTR Field Definition File and are summarized in the table below.

Notes for v1b: IRISTR_v1b includes minor structure changes/modifications and the new **STRUCTURE_InChIKey** field (25 character abbreviated InChI for use in structure-indexing applications) added as a DSSTox Standard Chemical Field to all DSSTox files.

EPA IRIS Website Search Categories & Column Headers	DSSTox IRISTR_v1a Field Names	New DSSTox Field Note
Oral RfDs	**Oral_RfD_Assessed**	*Counter field added by DSSTox*
Critical Effects	**Oral_RfD_CriticalEffects**	
Oral RfD	**Oral_RfD_mg_per_kg_day**	
	Oral_RfD_mmol_per_kg_day	*added mmol units*
Point of Departure(s)	**Oral_RfD_Notes**	*also includes footnotes and multiple values*
Overall Confidence	**Oral_RfD_Confidence**	
Inhalation RfCs	**Inhalation_RfC_Assessed**	*Counter field added by DSSTox*
Critical Effects	**Inhalation_RfC_CriticalEffects**	
Inhalation RfC	**Inhalation_RfC_mg_per_m3**	
	Inhalation_RfC_mmol_per_m3	*added mmol units*
Point of Departure(s)	**Inhalation_RfC_Notes**	*also includes footnotes and multiple values*
Overall Confidence	**Inhalation_RfC_Confidence**	
Weight of Evidence Characterizations	**WtOfEvidence_Cancer_Assessed**	*counter field added by DSSTox*
	WtOfEvidence_Cancer_Concern	*field added by DSSTox*
WOE 86 Guidelines	**WtOfEvidence_1986GuidelineCategories**	
	WtOfEvidence_UpdatedGuidelinesUsed	*field added by DSSTox*
WOE Narrative	**WtOfEvidence_Cancer_Narrative**	
Oral Slope Factors/Drinking Water Unit Risks	**DrinkingWater_OralSlope_Assessed**	*counter field added by DSSTox*
Precurser Effect/Tumor Type	**DrinkingWater_PrecursorEffect_TumorType**	
Oral Slope Factors	**DrinkingWater_OralSlopeFactor_mg_per_kg_day**	
	DrinkingWater_OralSlopeFactor_mmol_per_kg_day	*added mmol units*
Extrapolation Method	**DrinkingWater_ExtrapolationMethod_Notes**	*also includes footnotes and multiple values*
Drinking Water Unit Risks	**DrinkingWater_UnitRisk_microg_per_L**	
	DrinkingWater_UnitRisk_micromol_per_L	*added micromol units*
Study Route	**DrinkingWater_StudyRoute**	
Air Unit Risks	**Inhalation_UnitRisk_Assessed**	*counter field added by DSSTox*
Precurser Effect/Tumor Type	**Inhalation_PrecursorEffect_TumorType**	*"Air" changed to "Inhalation" on recommendation of EPA IRIS Group*
Air Unit Risks	**Inhalation_UnitRisk_microg_per_m3**	
	Inhalation_UnitRisk_micromol_per_m3	*added micromol units*
Study Route	**Inhalation_StudyRoute**	
Extrapolation Method	**Inhalation_ExtrapolationMethod_Notes**	*also includes footnotes and multiple values*
	TotalAssessments	*counter field added by DSSTox*
	Note_IRISTR	*note pertaining to a few DSSTox and IRIS CAS differences*
	Website_URL	*field added by DSSTox*

orange cells: IRIS website main search categories
blue cells: Fields added to DSSTox IRISTR file

Log of SDF Modifications and Version/revision updates:

Date	DSSTox SDF File Names	Modifications from previous version	Additional Notes
10Apr2006	IRISSI_v1a_544_10Apr2006	Initial launch publication of Structure-Index Locator file containing DSSTox Standard Chemical Fields and chemical-specific URLs for IRIS substance QuickView document web pages, but no additional Source toxicity data fields.	
28Jul2007	IRISTR_v1a_544_28Jul2007	Initial launch publication of modified version of IRISSI_v1a_10Apr2006, expanded to include 3 DSSTox Standard Toxicity Fields and 34 Source-specific toxicity data fields generated from the EPA IRIS Source website (listed in above table). Revised DSSTox Standard Fields from IRISSI_v1a_10Apr2006: **DSSTox_SID** has been replaced by two new ID fields **DSSTox_RID** and **DSSTox_Generic_SID**. **DSSTox_ID_FileName** has been replaced by new ID field: **DSSTox_FileID**. Entries in **TestSubstance_Description** field have been simplified. Entries in **ChemicalNote** that pertained specifically to IRISTR have been moved to Source-Specific field: **Note_IRISTR**	IRISTR is considered a "companion" database meaning that it is linked to and complements the content of an actively updated Source website. Periodic updates in this file will incorporate changes or additions to content provided on the EPA IRIS Source website. At the time of this publication, there were 4 substances with discrepancies between the DSSTox IRISTR CASRN and the EPA IRIS website CAS (information included in **Note_IRISTR** field): 1. Avermectin B1: DSSTox uses CASRN [71751-41-2] for mixture of B1a and B1b; IRIS CASRN [65195-55-3] is for Avermectin B1a. 2. Dalapon, sodium salt: DSSTox uses CASRN [127-20-8] for sodium salt; IRIS CASRN [75-99-0] is for parent. 3. Hexachlorodibenzo-p-dioxin (HxCDD), mixture of 1,2,3,6,7,8-HxCDD and 1,2,3,7,8,9-HxCDD: DSSTox uses CASRN [NOCAS]; IRIS lists two CAS for components of 2:1 mixture 1,2,3,7,8,9 HxCDD [19408-74-3] and 1,2,3,6,7,8-Hexachlorodibenzo-p-dioxin [57653-85-7]. 4. Percholorate and Perchlorate Salts: DSSTox uses CASRN [14797-73-0] perchlorate ion; IRIS CASRN [7790-98-9] is for the ammonium salt.
15Feb2008	IRISTR_v1b_544_15Feb2008	1 structure modified. New Standard Field added: **STRUCTURE_InChIKey** Modified field name: **Website_URL** changed to **ChemicalPage_URL**	All corrections or changes to structure information noted in **Note_IRISTR** field, searchable by version (e.g., v1b).

IRISTR SDF Content	Totals_v1a	Totals_v1b
# Records	544	544
DSSTox Standard Chemical Fields	18	19
DSSTox Standard Toxicity Fields	3	3
IRISTR Source Fields	34	34
Total # Fields	55	56
Chemical Content	**Counts_v1a**	**Counts_v1b**
STRUCTURE_ChemicalType:		
defined organic	465	465
inorganic	57	57
organometallic	17	17
no structure	5	5
STRUCTURE_TestedForm_DefinedOrganic:		
parent	449	449
complex	5	5
salt	11	11
salt complex	0	0
TestSubstance_Description:		
single chemical compound	495	495
mixture or formulation	32	31
unspecified or multiple forms	17	18
macromolecule	0	0

IRISTR Toxicity Review Areas*	Totals_v1
Oral RfDs	357
Inhalation RfCs	70
Weight of Evidence Characterizations	243
Oral Slope Factors/Drinking Water Unit Risks	76
Air Unit Risks	54
Total Assessments	800

***** 357 IRIS chemicals have an "Oral RfD" Toxicity Review assessment; 70 have an "Inhalation RfC" Toxicity Review assessment, etc.

Number of IRISTR Toxicity Review Assessments per Chemical**	Totals_v1
0	(39)
1	323
2	101
3	54
4	22
5	5
Total Assessments	800

** 39 IRIS chemicals have 0 Toxicity Review assessments; 323 IRIS chemicals have 1 Toxicity Review assessment, etc.